Applying CMAQ/Models3 for Air Toxics Assessments

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Motive

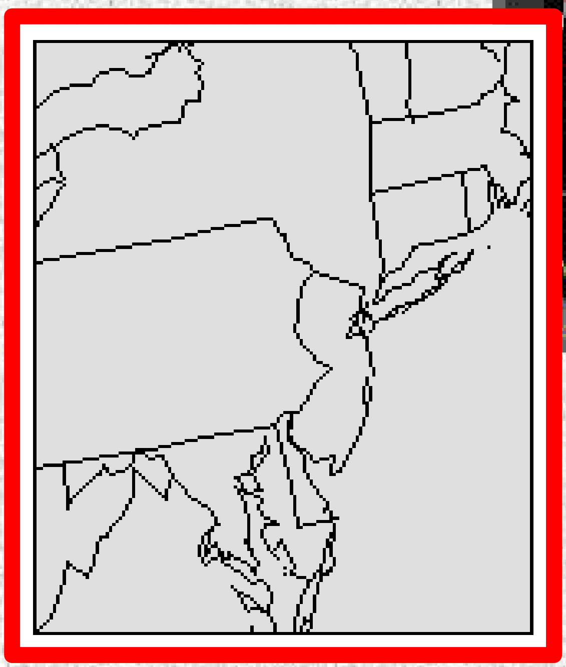
Many air toxics depend on processes not treated by standard regulatory models.

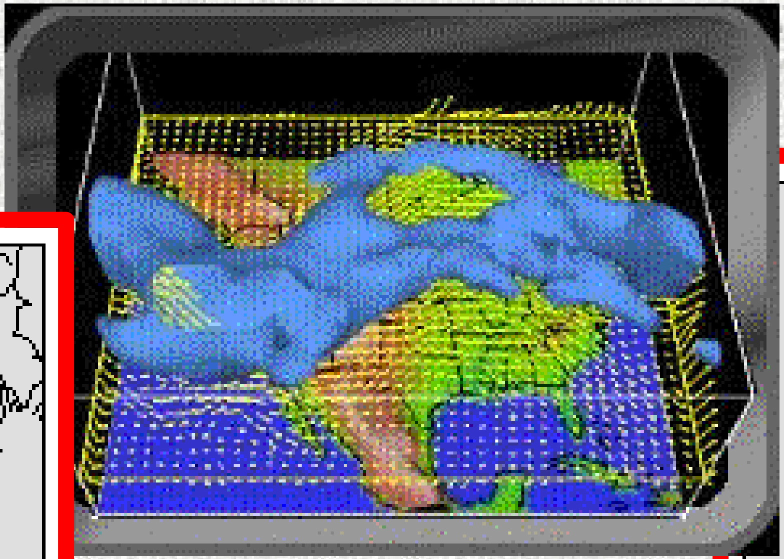
- Meteorological
  - ✍Long Range Transport (>50 Km)
  - ✍Complex Vertical Mixing and Deposition
- Physical
  - ✍Gas to Aerosol Exchange
  - ✍Scavenging by Cloud Droplets
- Chemical
  - ✍Secondary Production
  - ✍Transformation with Cloud Droplets

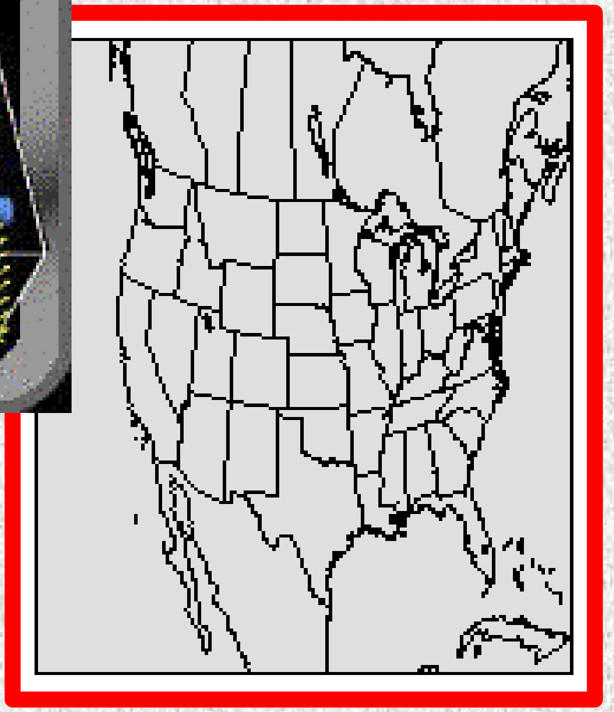
Many standard models cannot simultaneously treat these process multiple sources

Motive (Cont.)

- Can we adapt an existing model to assess the fate of such compounds?
- The model would simulate spatial domains and processes as below.

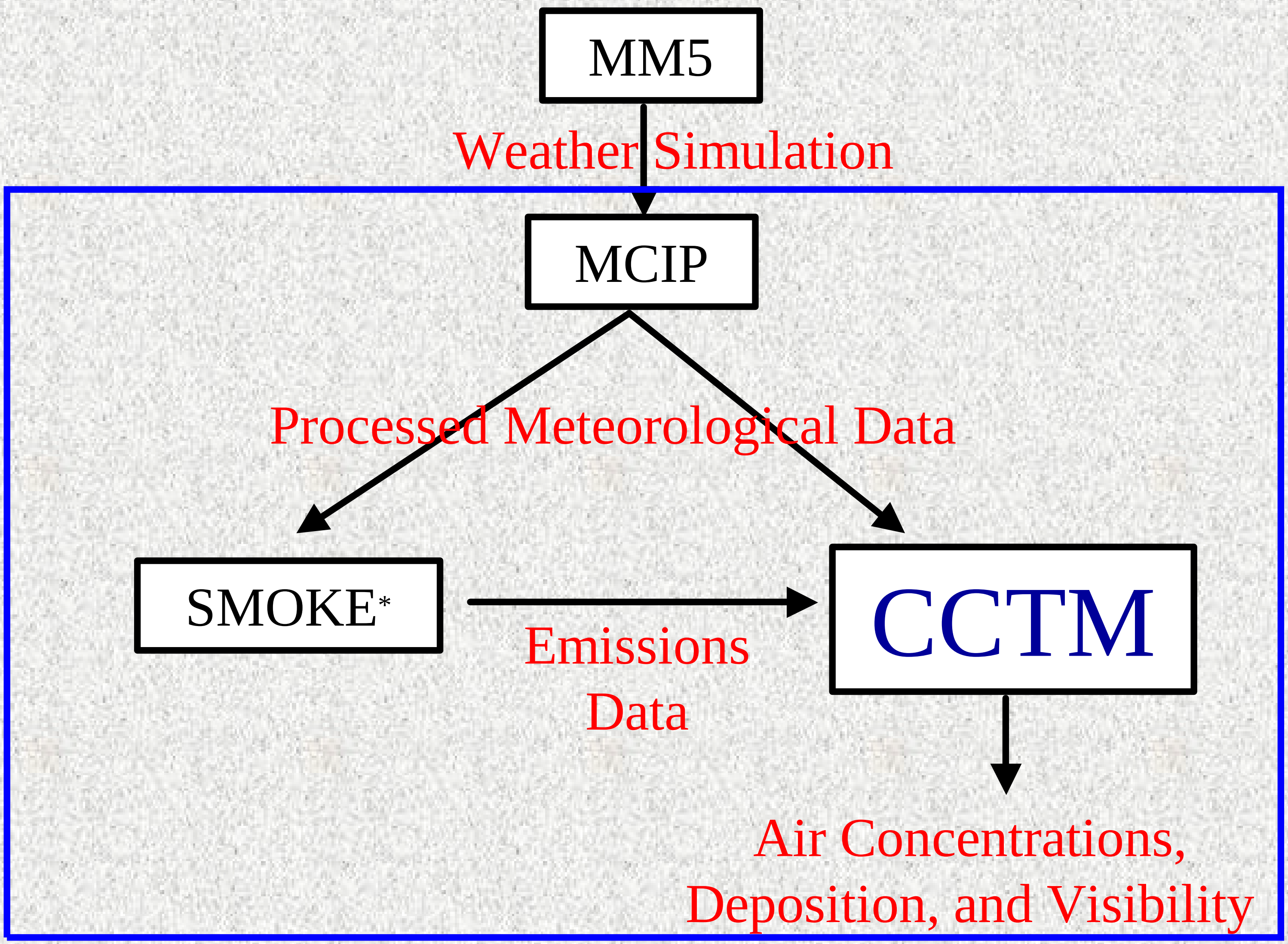






Community Multiscale Air Quality (CMAQ) system

- Eulerian-based modeling system
- Simulates urban and regional Scale transport, and chemical processes
- Applies the “One-Atmosphere” approach for Air Quality and Deposition Modeling
  - Atmospheric Radicals (i.e., O_3, VOC’s, $NO_{X.}$, etc.)
  - Atmospheric Aerosols (i.e., composition, size distribution, etc.)
  - Deposition (Sulfate, Nitrate, etc.)



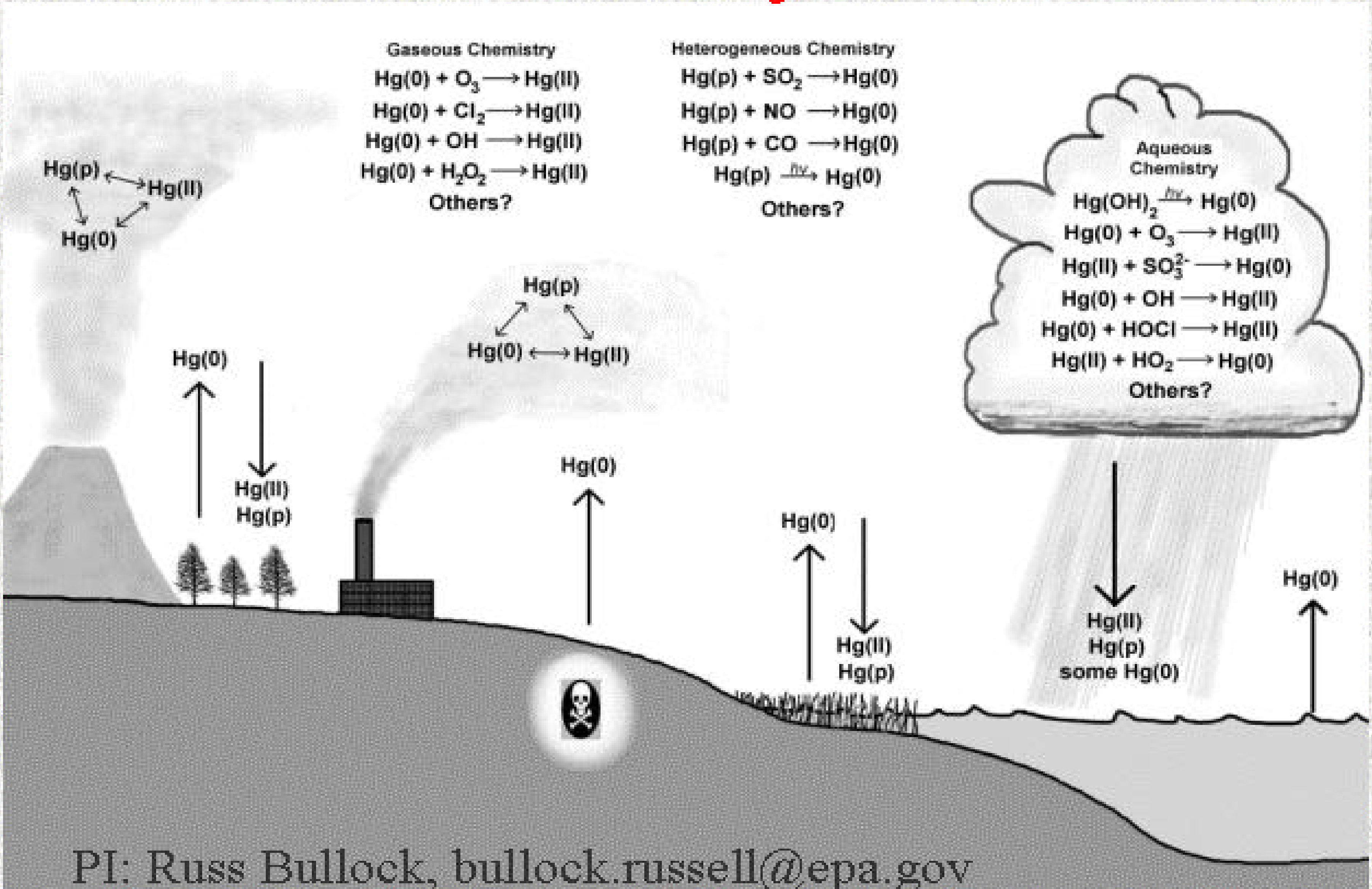
Dashed Box encompasses
CMAQ/Models3 Elements

*SMOKE is a product of the MCNC.

Current Projects of CMAQ for Toxics

- Continental-Regional Studies
  - Atmospheric fate modeling of emissions
  - Air concentrations and depositions
  - National and Regional Assessments
- Research Studies
  - Develop tools
  - Assess processes controlling air toxics
  - Simplify environmental assessments

Mercury



PI: Russ Bullock, bullock.russell@epa.gov

Overview

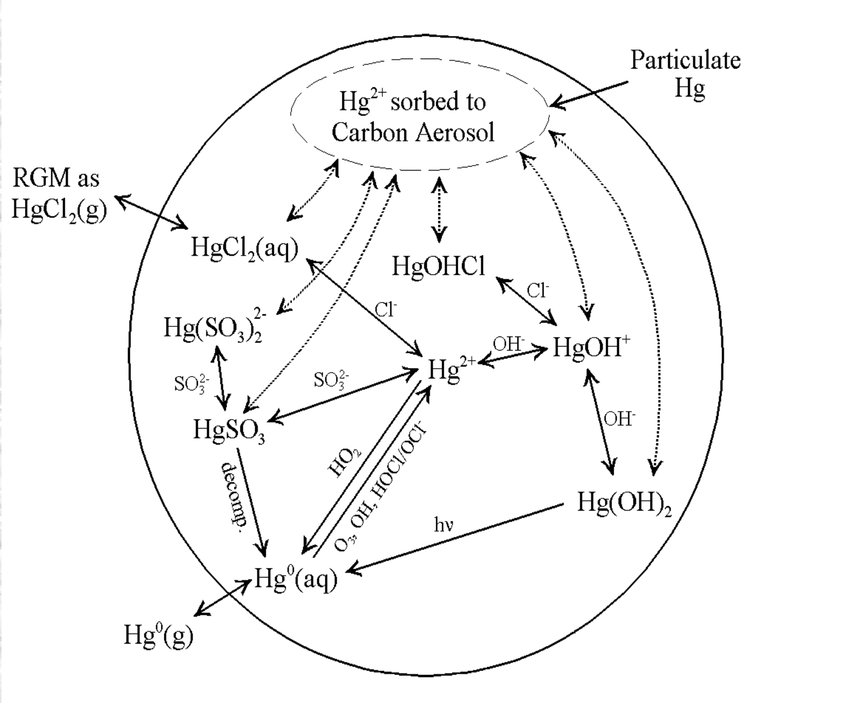
- Expand gas and aerosol species
  - Elemental Mercury, Hg(0)
  - Reactive Gaseous Mercury, RGM or Hg(II)
  - Particulate Mercury, Hg(P)

- Adapt Cloud Chemistry

- Include Gas Chemistry

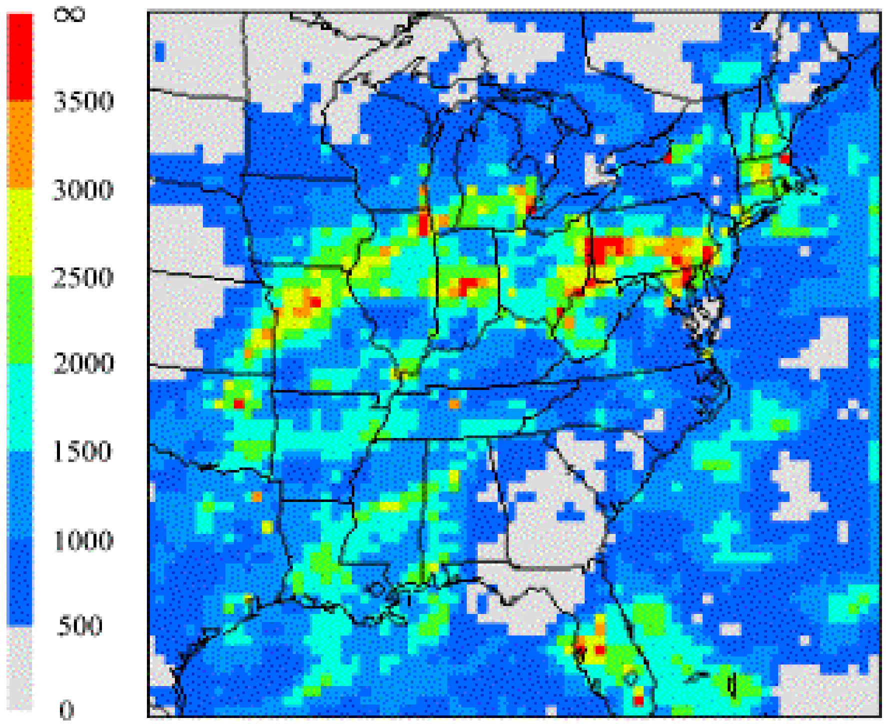
  Hg(0) ✍ RGM

  Hg(0) ✍ Hg(P)

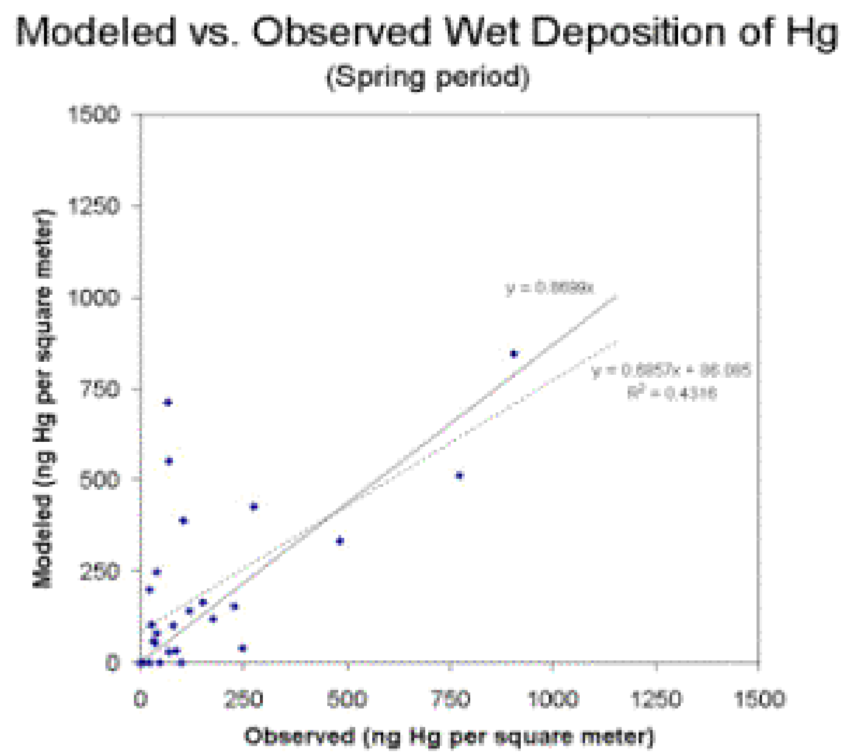


Test and Results

- CMAQ-Hg simulations performed for spring and summer periods in 1995
- Simulated wet deposition compared to observations from the Mercury Deposition Network

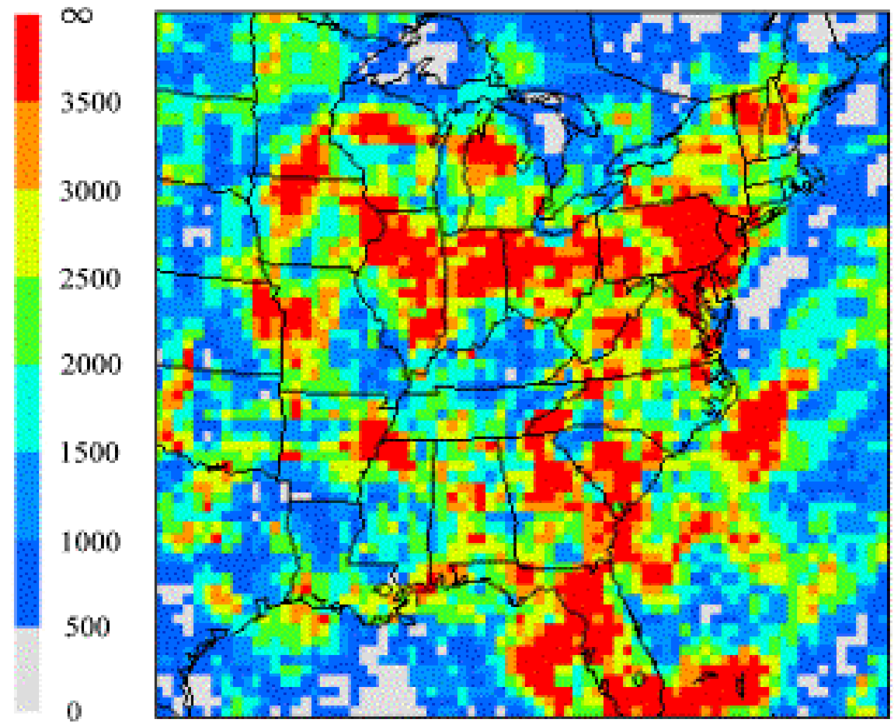


Spring Period 1995: Predicted Wet Deposition

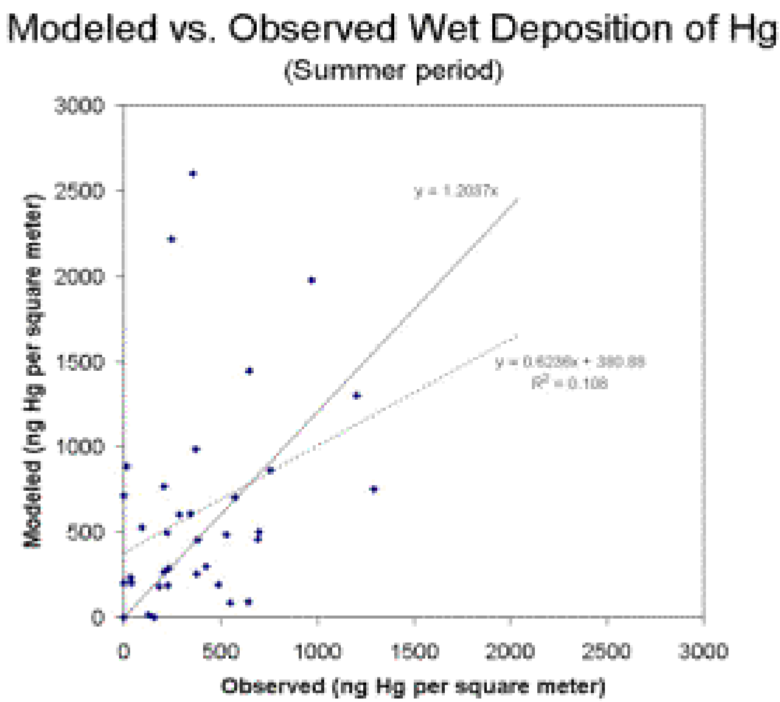


Atm. Env. **(2002), Vol. 36, Issue 13, pages 2135-2146.**

Results (Cont.)



Summer Period 1995: Predicted Wet Deposition



***Atm. Env.* (2002), Vol. 36, Issue 13, pages 2135-2146.**

General CMAQ-Hg Test Results

- ✍ Simulated cloud chemistry agrees with most other models within a factor of two, but there remain questions about the strong diel cycle it exhibits.
- ✍ Cloud water model produces total Hg concentrations that are within the range of observed values, but observational data on cloud water loading versus air concentrations of the various forms of Hg are lacking.
- ✍ Full-scale model results for wet deposition are strongly dependent on the validity of the precipitation definition.
- ✍ Model behavior for mercury wet deposition is comparable to that seen in RADM sulfur modeling in the mid-1980's; accuracy was moderate in cool seasons, but poor when convective precipitation is prevalent.
- ✍ More comprehensive testing is certainly needed.

Select Volatile Hydrocarbons

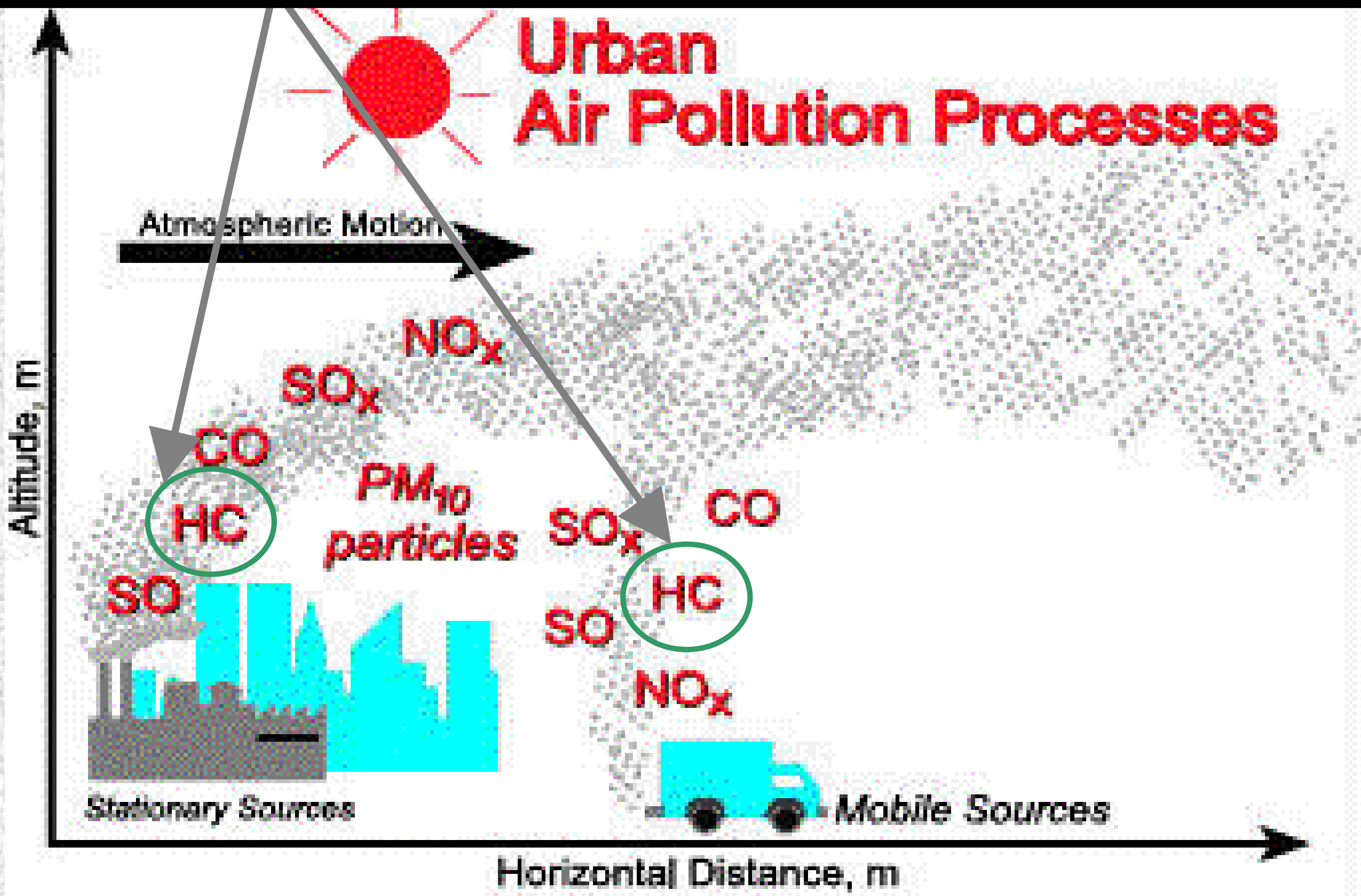


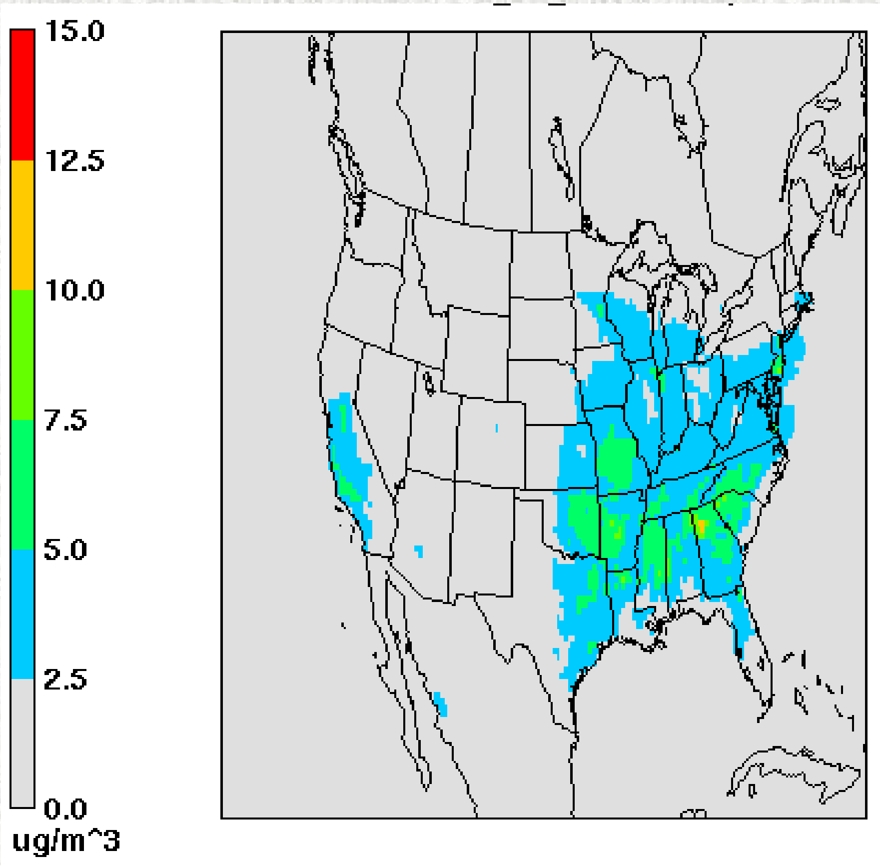
Figure Courtesy: NIEHS/NIH

PI: Jerry Gipson, ggb@hpcc.epa.gov

Context

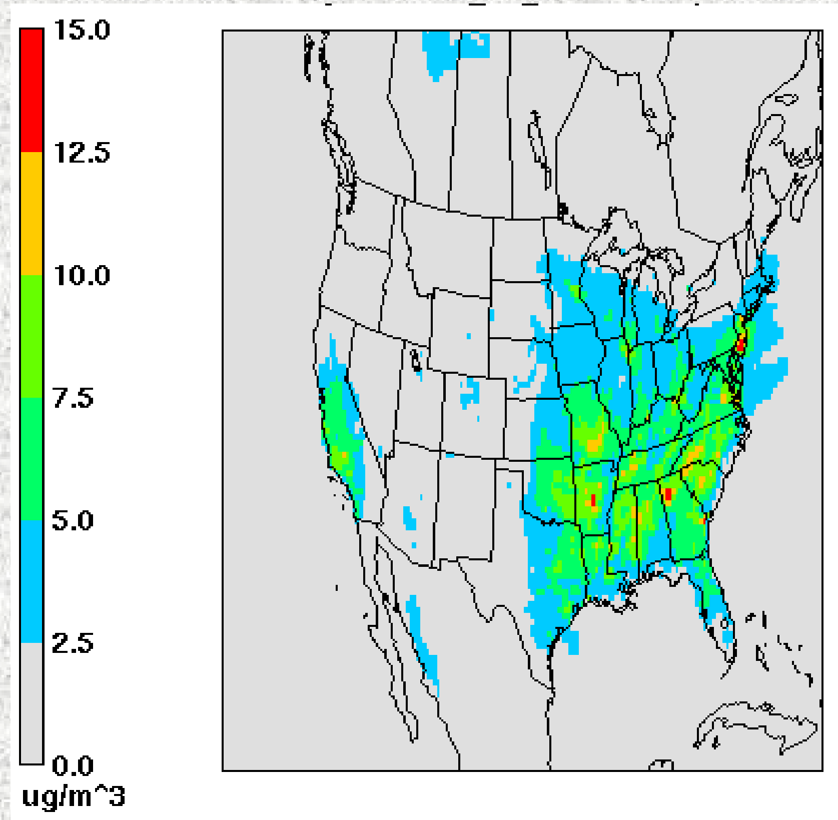
- Simulate VOC's labeled as air toxic
  - Benzene
  - Formaldehyde
  - Acetaldehyde
- Adapt chemistry mechanism for Ozone
  - Sought compound implicitly represented
  - Step toward diurnal loss and production
- Support the 1999 National Air Toxics Assessment (NATA)
  - Annual Assessments
  - Continental Domain

Formaldehyde from SAPRC99

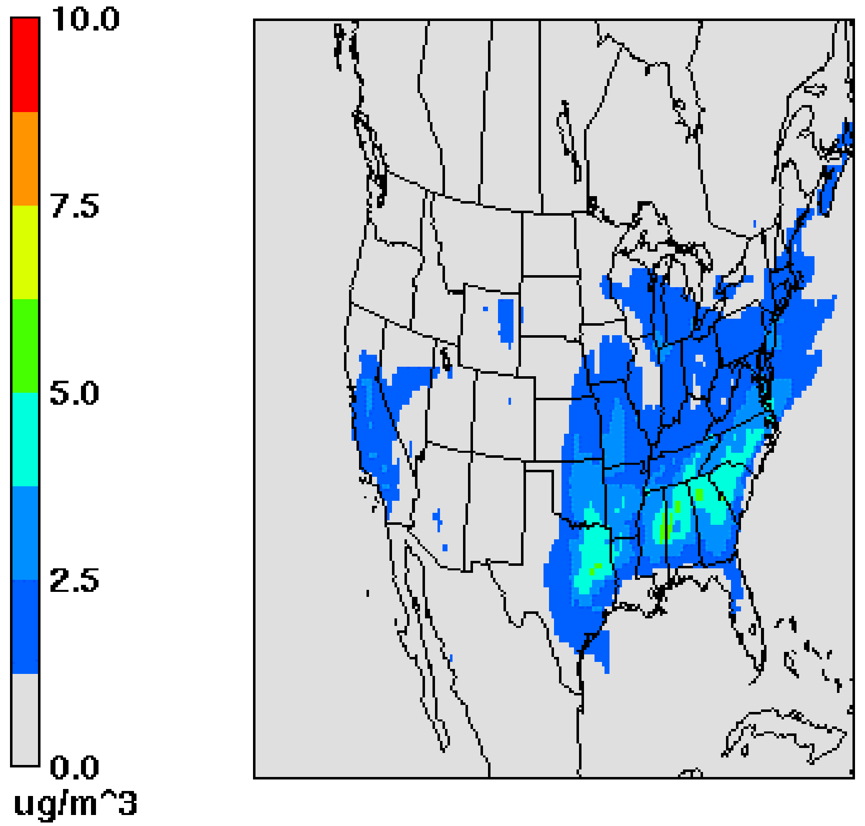


HCHO, Daily Average:
July 8, 1999

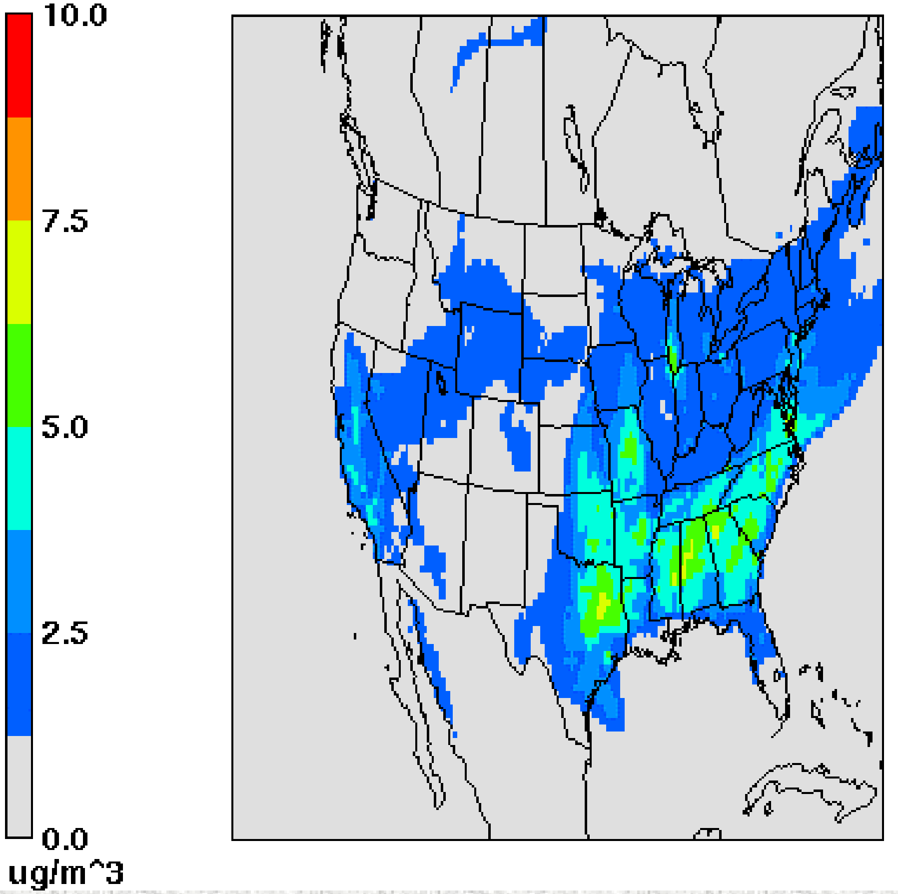
HCHO, Hourly Maximum:
July 8, 1999



Acetaldehyde from SAPRC99

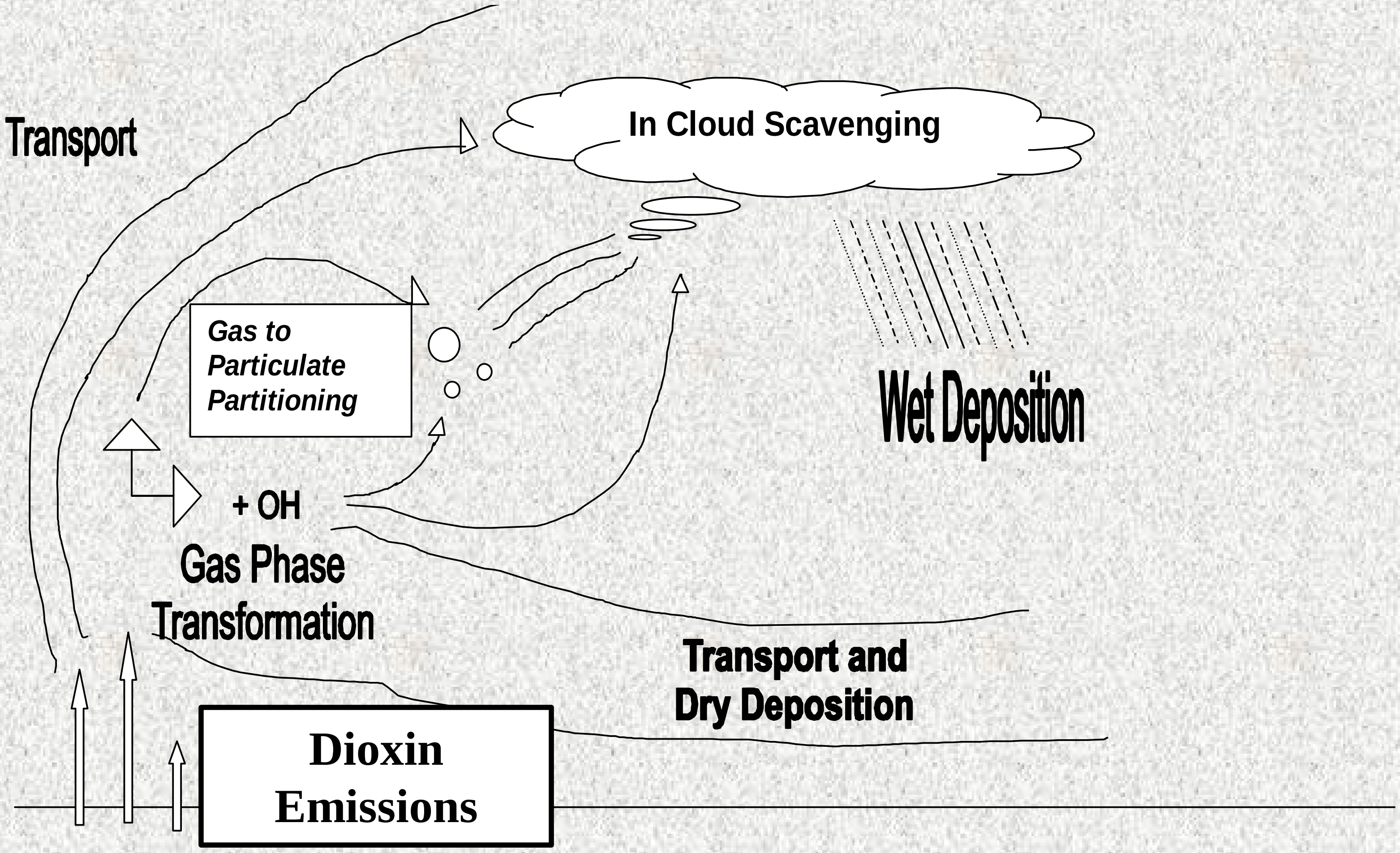


CH_3CHO, Hourly Maximum:
July 8, 1999



CH_3CHO, Daily Average:
July 8, 1999

Toxic Dioxins and Furans



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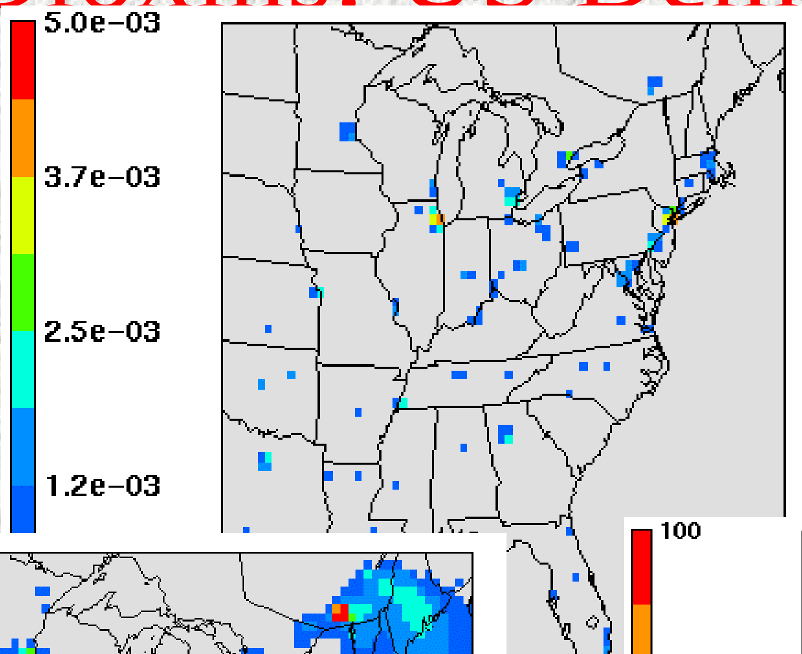
Overview

- 17 Polychlorinated Dibenzo-p-Dioxins and Dibenzo Furans
  - Significant toxicity on WHO and NATO scales

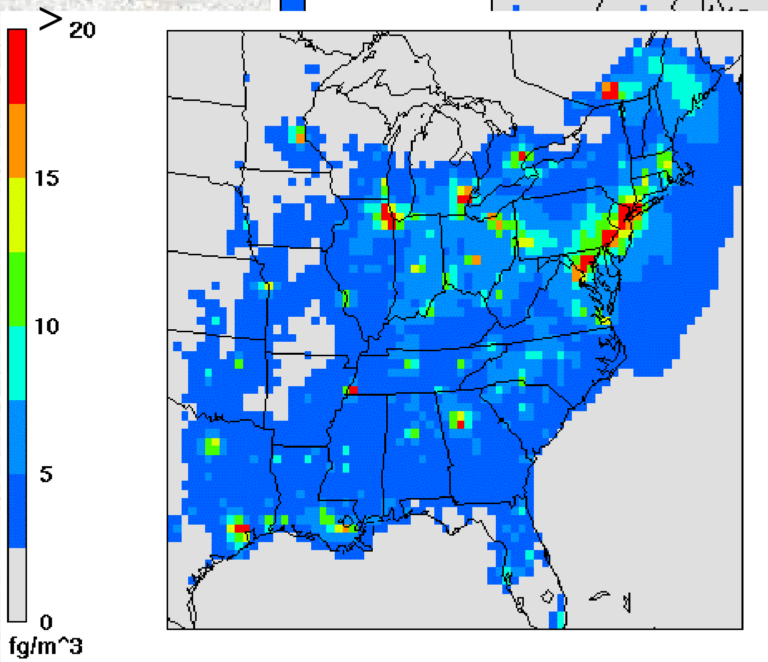
- Major challenges:
  - Expand Chemical and Aerosol Species
  - Include Chemical Loss Process
  - Simulate the gas to aerosol exchanges
  - Obtain reliable emissions data

- Support NATA for 1999
  - Air concentration and deposition over the US
  - Final Result in terms of TEQ

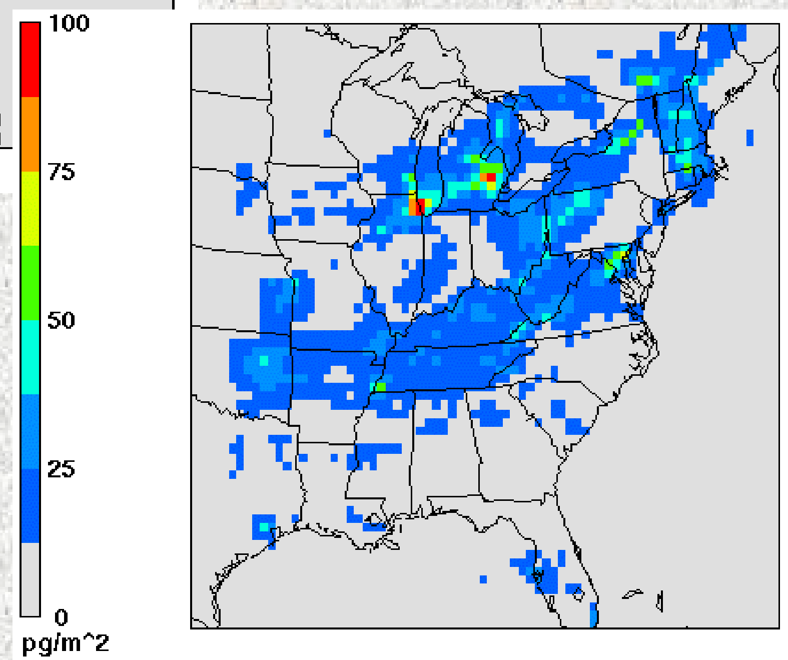
Dioxins: US Demonstration



TEQ-I Emissions Scenario: Average gm/hr Emissions, Mid to Late April 1995

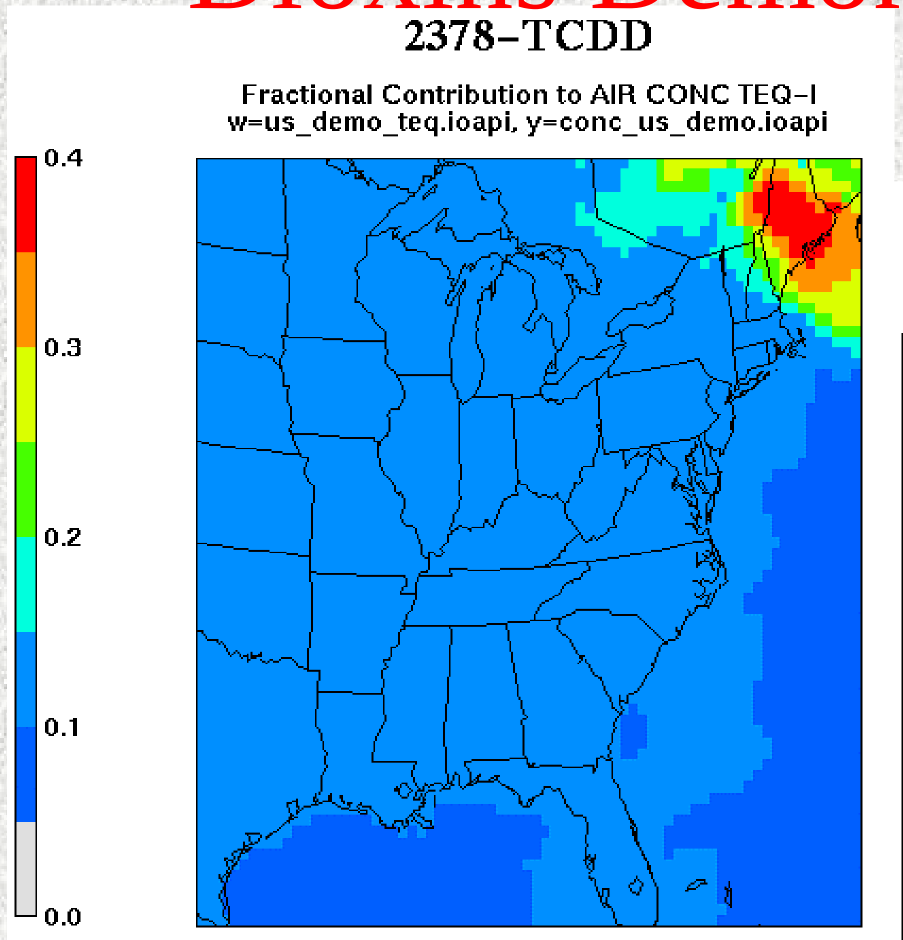


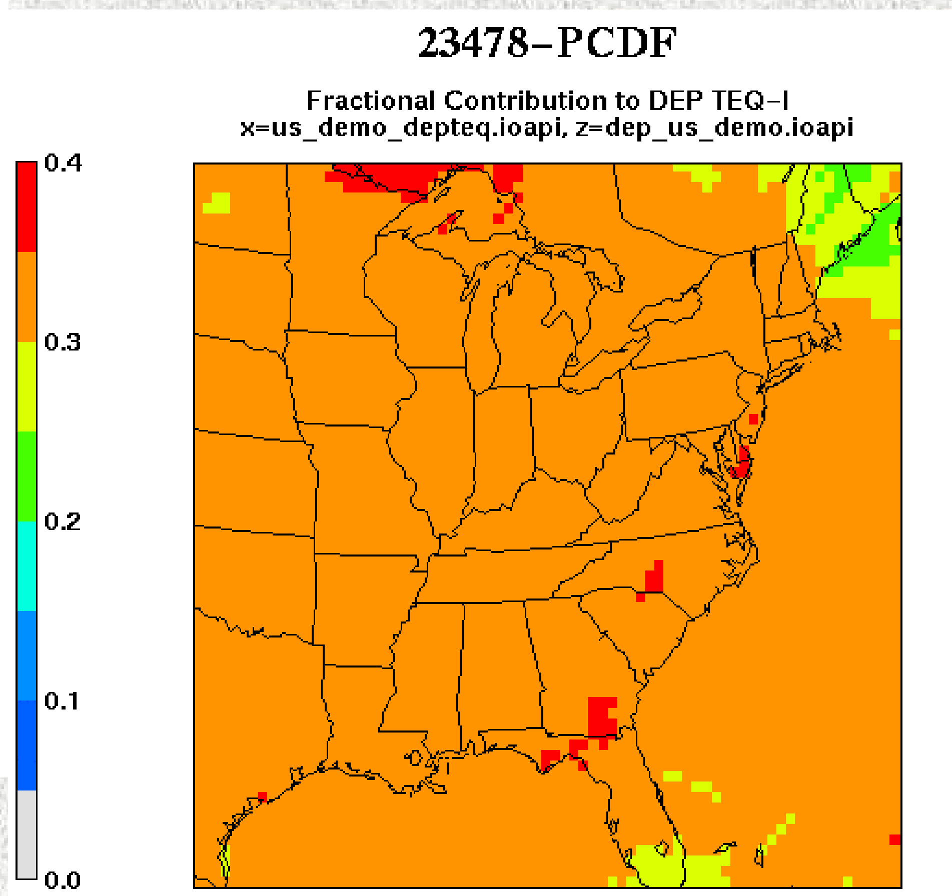
Predicted Average Air Concentration in TEQ-I



Predicted Total Deposition in TEQ-I

Dioxins Demonstration (Cont.)





Model does treated congeners individually. Output can tell how each congener contributes to TEQ-I.

Neighborhood Modeling of Urban Air Toxics

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Overview

- Use modeled air quality to support human exposure models such as SHEDS
- Obtain outputs such as
  - fields of air concentration
  - statistic distributions describing sub-grid concentration variability (PDFs)
  - range of urban morphologies
- Development modeling tools for neighborhood scales

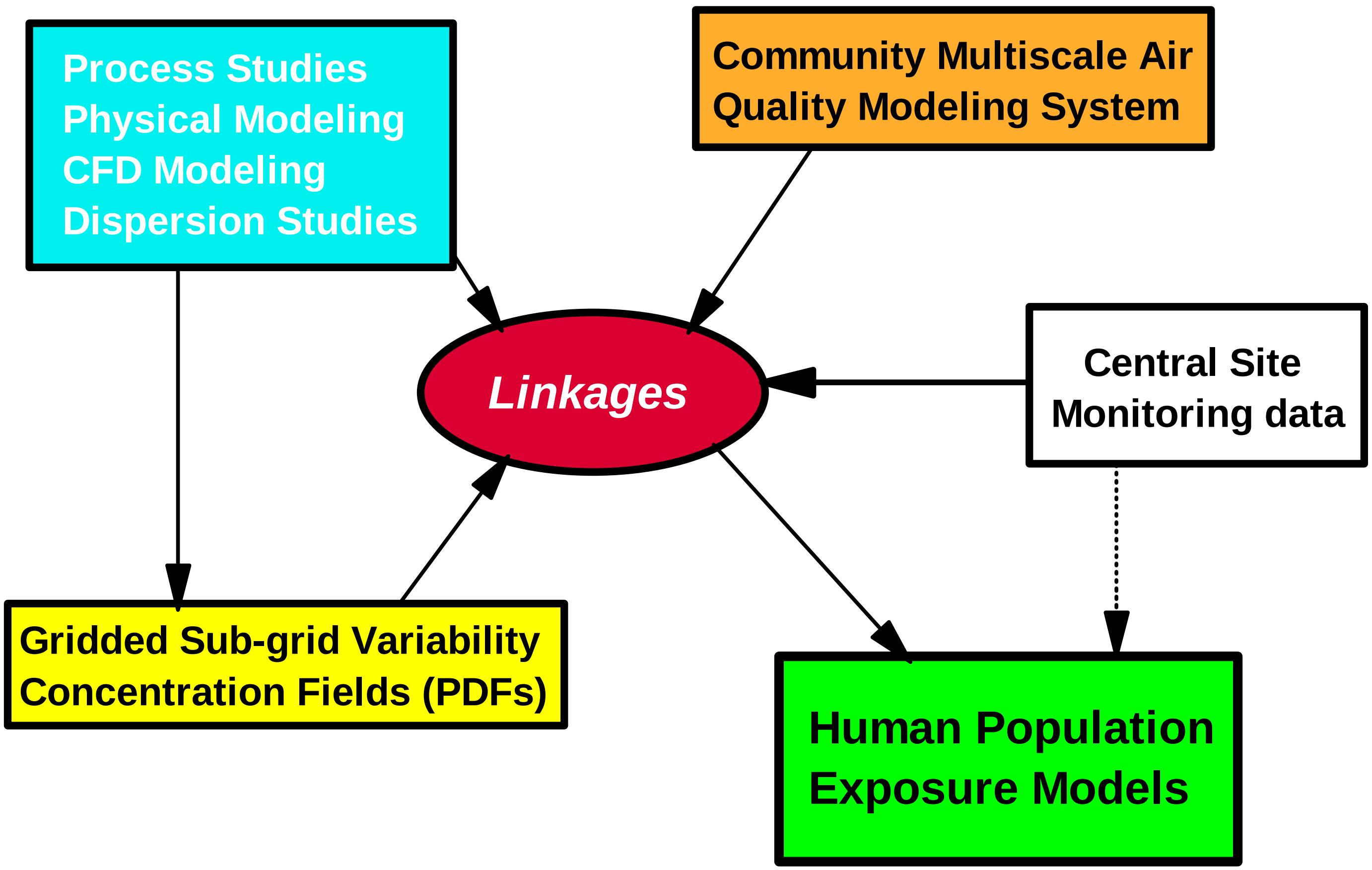
Challenges

- Grid and sub-grid resolutions appropriate for separate pollutants or groupings
- Convolution of multiple sources within urban environment
- Impacts from chemistry and physics such as secondary production and aerosol microphysics
- Concentration statistics for assessing human exposure

Status and Plans of Project

- **Develop and parameterize urban canopy**
- **Designate urban morphology classes**
- Develop probability distributions functions for sub-grid variability Off line (CMAQ post processor)
  - Parameterize the dispersion functions
  - Handling concentration singularities (x=0)
  - Linkages to urban morphology
  - On-line into MM5 (long term)
- **Apply in prototype study for Philadelphia**
- **Cooperate with studies for Houston**
- Verify with more sophisticated techniques such as for Physical and CFD modeling

Project



Process Studies
Physical Modeling
CFD Modeling
Dispersion Studies
Community Multiscale Air Quality Modeling System
Linkages
Central Site Monitoring data
Gridded Sub-grid Variability Concentration Fields (PDFs)
Human Population Exposure Models

Summary

Presented Applications obviously support air quality and exposure assessments.

- NATA
- Control Strategies

They indirectly support the above assessments.

- Boundary Conditions
- Tools Development
- Integrated Risk Estimates

Other application simply and improve assessment.

- Identify key process controlling specific air toxics.
- Check simplifications to modeling these processes

Future Development Projects

Address thirty-three compounds emphasized by NATA

Specific toxics that could be addressed

- Inert and involatile metals
- Halocarbons
- Acrolein

For more information about CMAQ, go to
http://www.epa.gov/asmdnerl/models3/CMAQ/index.html